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RESEARCH ARTICLE

Mathematical concepts for the micro-mechanical modeling of
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This contribution reviews mathematical concepts of micro-mechanical modeling in the phase-field approach applied to dislocation dynamics. The intention is twofold: On the one hand, modelling of dislocation dynamics is a very recent field of development in phase-field theory, in comparison to the simulation of diffusional phase transformation and related micro-structure evolution problems in materials science. The reason is that modelling dislocation dynamics poses several challenge for phase-field concepts which go beyond purely diffusional problems in materials science as, e.g., dendritic solidification, as we point out in Sect. 3. On the other hand, the modelling of dislocations has triggered further wide-ranging developments of phase-field based models for deformation problems. This is an important development, since a comprehensive model for deformation problems should include dislocation as well as diffusional degrees of freedom from the atomic scale to the microscale. This is something phase-field theory is capable of, as discussed in this review article. We aim to give an overview on relevant mathematical concepts, and to stimulate further steps in this direction.

1. Introduction

We start by considering a representative problem of deformation dynamics for materials, namely that of precipitate microstructure evolution in superalloys, such as, e.g., Ni-based superalloys [1–3]. In this example, it is the impedance of dislocation motion of intermetallic precipitates (precipitate hardening) which is the dominant mechanism governing the superalloys' high strength. Additionally diffusive processes such as chemical ordering can couple strongly to dislocation shearing processes in governing the rate of deformation [3–5]. As Wang and Li point out in their recent review *Phase-field modeling of Defects and Deformation* [3], on the other hand dislocation plasticity can also change the precipitate microstructure morphology in form of an instability called ratering, where the precipitate morphology changes from an initial cuboidal shape to a plate respectively a rod shape [6–10]. Thus the overall dynamical problem is one of mechano-chemically or dislocation-diffusional coupled mechanisms, where microstructure evolution as, e.g., grain growth, precipitate evolution or solute segregation, goes hand in hand with mechanical deformation. This is a difficult problem to model using a purely mechanical approach, even though it is a representative problem of deformation dynamics [11]. Now phase-field modeling has already established itself in modeling microstructure evolution with interfaces

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to free-energy and mobility databases (see, e.g., [3] and references therein), so it appears to be a plausible and valuable step to integrate deformation modeling in its framework. Since a mathematical concept for dislocation dynamics is the first step to do so, this is our focus in this review. It is worth noticing in this context that the phase-field (PF) approach has recently been extended to the atomic scale in form of the phase-field crystal (PFC) approach, which can be coupled directly to the classic phase-field approach [12, 13]. This even allows to take into account the different time and length scales tied to the above representative problem in the manner depicted in Fig. 1.

How do we have to picture the methodological difference between the (classical) phase-field and the phase field crystal method such that the latter can be applied to the atomic scale? A typical example of an application of the phase-field (PF) method is solidification: Consider a material that is disordered at high temperature and has two stable phases at low temperature. Upon quenching the material from high to low temperature, grains of different stable phases will develop and evolve in competition with each other. Phase field modelling is able to describe the time evolution of such a process. To do so, a continuous function of space and time $\phi(r, t)$ is introduced — namely the phase field — which assumes a different constant value for both stable phases. Close to an interface between two grains, the value of ϕ changes rapidly. The phase field variable introduced in the context of this example can be interpreted as an order parameter to represent the relative mass fraction of both phases. It allows to model and simulate the dynamics of interfaces, which may change their topology during evolution in time — the so-called Stefan problem [14] — elegantly, i.e., without the need to track the interface explicitly.

Classic phase field models are based the following Landau form of a free energy functional

$$F = \int_V \left[\frac{\epsilon^2}{2} |\nabla \phi|^2 + f(\phi) \right] dV. \quad (1)$$

From (1), the dynamical evolution of the field equation can be derived via a variation and is found to be of form

$$\frac{\partial \phi}{\partial t} = \Delta \frac{\delta F_i}{\delta \phi} \quad (2)$$

or

$$\frac{\partial \phi}{\partial t} = - \frac{\delta F_i}{\delta \phi}, \quad (3)$$

depending on whether ϕ can be assumed to be *locally conserved* (eq. (2)) respectively *locally non-conserved* (eq. (3)).

A functional of form (1) applies if the stable states of the system under investigation are locally uniform. If this assumption is not valid, an appropriate energy functional is given by

$$F = \int_V \left(\frac{1}{2} \phi [(q_0^2 + \Delta)^2 - \epsilon] \phi + \frac{1}{4} \phi^4 \right) dr, \quad (4)$$

now with two phenomenological parameters q_0 and ϵ . Again an equation of motion can be derived based on a variational principle, as for (2). This results in the simplest

formulation of the so-called phase-field crystal method, a recent extension of the phase field method to the atomic scale, originally derived in [15]. It is motivated by the Swift-Hohenberg equation [16], formulated to describe systems where the stable states are periodic, as, e.g., it is the case for Rayleigh-Bénard convection. Since its introduction, the phase-field crystal (PFC) method [15, 17–20] has emerged as a computationally efficient alternative to molecular dynamics (MD) simulations for problems where atomic and continuum scales are tightly coupled. The reason is that PCF operates on atomic length scales and diffusive time scales. Thus for a simple application, such as diffusion in gold or copper, it runs 10^6 - 10^8 times faster than the corresponding MD calculation [21]. In that sense it provides from point of view of multiscale materials modeling an interesting link between the phase-field method and MD. Moreover, a connection between classical density functional theory of freezing and phase-field crystal modeling could be identified in [18]. Thereby a second theoretical foundation besides the Swift-Hohenberg amplitude equation approach could be established. Essentially, it motivates the application of PFC models also for spatially non-uniform *non-periodic* states. See Section 4 for an overview of PCF.

Comparing the phase-field approach and the phase-field crystal approach sketched above, it seems that it is exactly the concept of a phase-field which appears promising to tackle challenges in modelling deformation problems which demand a comprehensive model concept, including displacive as well as diffusional degrees of freedom from the atomic scale to the microscale. The aim of this review is to collect some relevant mathematical methods, and to stimulate further steps in this direction. The article is organized as follows: In Section 2 we review the basic concepts of phase-field modelling, related to the interpretation of the diffuse interface model description which it yields. In Section 3 we explain first the challenges posed by dislocation modelling for phase-field concepts before turning to a review of the various models based on this concept. The latter have been established to simulate the dislocations themselves, the associated microstructure, the dynamics of both as well as their interaction with other structures of the respective material. Finally, we conclude with an outlook on multiscale modelling of dislocation dynamics involving the phase-field and the phase-field crystal approach.

2. The basic concept of phase-field modelling

If one does not take solely a materials science point of view, but understands phase-field modeling rather as an important concept to model condensed matter systems in general, then it applies to inhomogeneous systems which involve domains of well-defined phases separated by a distinct interface — just as one can picture the different kinds of small-scale structure in materials science. If such systems are driven out of equilibrium, one phase will grow at the cost of the other. Examples are phase separation by spinodal decomposition or nucleation and subsequent growth of the nucleus in the nourishing phase [22]. Another example which has often been discussed as a paradigmatic problem is that of dendritic solidification [23–26]. A phenomenological description involves the definition of a precisely located interfacial surface where boundary conditions are imposed. One of those boundary conditions typically yields the normal velocity at which the interface is moving. This is the so-called *sharp interface* approach, adopted both in analytical and numerical studies for a variety of contexts involving a moving boundary. The origin of such a description is often transparent, being obtained by symmetry arguments and common sense as well as considerations of mass and energy conservation. Nevertheless, the properties of sharp interface models can be quite subtle as in the

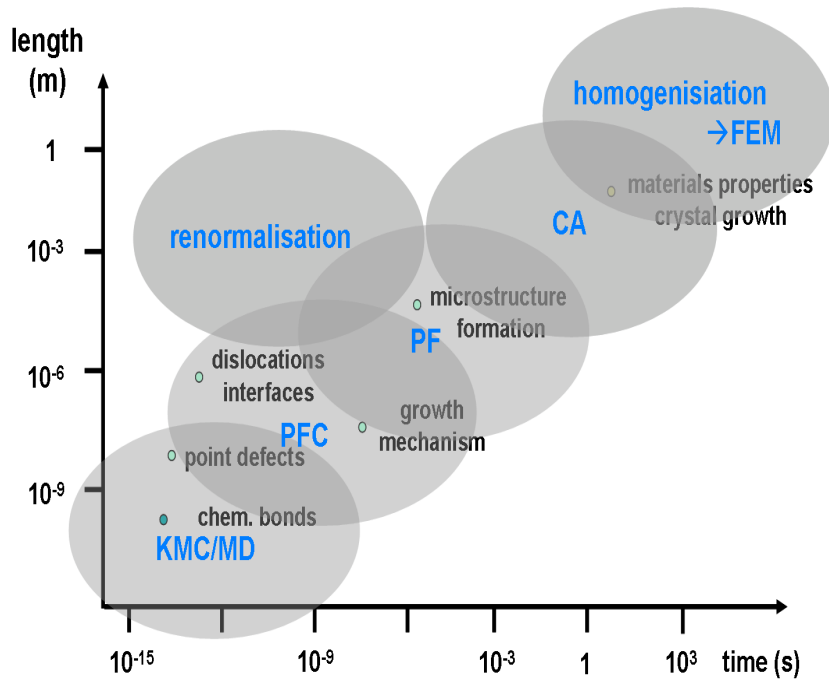


Figure 1. Schematic plot of the multi-scale challenge of computational materials design; Shown are different scales relevant to dislocations, in particular the phase-field (PF) and the phase-field crystal (PFC) modelling approach.

case for dendritic growth. This is strongly coupled to the question of how to view the interfacial surface. Already when introducing the notion of a surface quantity, Gibbs implicitly entertained the idea of a diffuse interface [27]: any density of an extensive quantity (e.g., the mass density) between two coexisting phases varies smoothly from its value in one phase to its value in the other. The existence of a transition zone, though microscopically of atomic extent, underlies this definition of surface quantities as given by Gibbs. In phase transition phenomena, this notion has been employed in the spirit of Landau and Khalatnikov [28], who were the first to introduce an additional parameter — i.e., a *phase-field* — to label the different phases in their theory on the absorption of liquid helium. Essentially phase-field modelling, as it appeared subsequently in the literature in the context of phase transition phenomena [29, 30], is connected to such an additional order parameter. Clearly such models have advanced the numerical treatment as well as the general understanding of interfacial growth phenomena since then.

Even though quite a young approach to tackle such problems, phase-field models have been employed by different groups in rather different spirits. One might even be tempted to say that a variety of philosophies accompanying phase-field modelling coexist.

One way to view this method to model interfacial growth is to understand it as a numerical technique, which helps to overcome the necessity of solving for the precise location of the interfacial surface explicitly in each time step of a numerical simulation, as achieved by the introduction of one or several additional phase-field variables. In such an approach the phase-field variables are continuous fields which are functions of space r and time t . They are introduced to describe the different relevant phases. Typically, these fields vary slowly in bulk regions and rapidly, on length scales of the order of the correlation length ξ , near interfaces. Here ξ is also a measure for the finite thickness of the interface. The free energy functional F determines the phase behaviour. Together with the equations of motion, this

yields a complete description of the evolution of the system. In other contexts, such as critical dynamics [22, 31, 32], the fields are order parameters distinguishing the different phases. In a binary alloy, for example, the local concentration or sub-lattice concentration can be described by such fields. The ideas involved in this approach have a long history, referring back to van der Waals [33, 34].

The materials science community associates the use of continuum field models in particular with the work of Cahn and collaborators [29, 35, 36]. Within their contribution to the field, phase-field models are more than just a “trick” to overcome numerical difficulties. Rather, they are rigorous derivations based on the variational principles of irreversible thermodynamics as founded by Onsager [37]. Then ensuring *thermodynamic consistency* of the model equations can serve as a justification of a phase-field model. In this sense, phase-field models can also be formulated for problems for which sharp interface equations are not yet available. Consequently, it might be their analysis which yields a formerly unknown sharp interface formulation and helps to clarify the physics in the interfacial region.

One has to contrast this procedure to a very established second way to validate a phase-field model. This second approach assumes that a given sharp interface formulation of the growth problem is the correct description of the physics under consideration. On the basis of this assumption, a phase-field model can be justified by showing that it is asymptotic to the correct sharp interface description, i.e., that the latter arises as the *sharp interface limit* of the phase-field model when the interface width is taken to zero. Obviously, this procedure works only for cases where a well established set of continuum equations describing the dynamics in the sharp interface formulation does exist. Moreover, if employed in this way, phase-field models do not seem to be of much help to elucidate the physics of the interfacial region beyond what is captured within the sharp interface model equations.

However, this is only partially true in the view of the third philosophy which has appeared in the phase-field community lately. It is rooted in the understanding of the finiteness of the interfacial surface in the sense of Gibbs discussed above: If one assumes a phase-field model to be thermodynamically consistent and to describe a physical situation for which an established sharp interface formulation exists as well, then, certainly, in the *sharp interface limit* the phase-field model should correspond precisely to that sharp interface formulation. However, keeping in mind that the interface can be understood to be of finite width, not only the *sharp interface limit* of a phase-field model is a meaningful physical limit, but also the so-called *thin interface limit* introduced by Karma and Rappel [38–40].

To clarify the difference between the *sharp interface limit* and the *thin interface limit*, we consider the growth of a dendrite with tip radius R in an undercooled melt [41]. Under more general circumstances, R might be representative of a typical macroscopic length scale such as the container size. For dendritic solidification at large undercoolings, the growth is rapid and the radius of curvature of the dendritic tip is relatively small. As a consequence, effects of capillary action and kinetics on the local interfacial temperature can be significant. In this regime, sharp interface limits of the phase-field equations have been calculated [42–47], which assume that the dimensionless interfacial temperature u is of the order of the small parameter ξ/R . Contributions from capillary effects and kinetics can be regarded to be of the same order. In this limit, one also considers ξ to be small compared to the capillary length l_c , which presents a stringent resolution requirement for a numerical computation that aspires to describe this limiting case. At low undercoolings, on the other hand, dendrites grow more slowly and have a larger radius of curvature, so that it is reasonable to model capillary effects and kinetics as small corrections. Karma and Rappel refer to the corresponding analysis as the *thin interface limit*.

For this thin interface limit one assumes $\xi \ll R$ but allows $\xi \sim l_c$. Almgren [48] has described this analysis as *isothermal asymptotics*, since to leading-order in ξ/R the temperature is isothermal throughout the interfacial region with $u = O(\xi/R)$. An extension to general non-isothermal multi-component alloy systems allowing for arbitrary phase diagrams with two phases was achieved only recently in [49], based on second order asymptotics.

Again, an interest in employing such an isothermal asymptotics or thin interface limit can be rooted in numerical considerations: the analysis can serve as a legitimization of a choice of model parameters which ensures an improved numerical performance. On the other hand, isothermal asymptotics can also be used to obtain first order generalisations of the well known Gibbs-Thompson relation, which usually yields the temperature at the interface. In turn, such a generalisation can facilitate subsequent stability analysis of the model.

Thus currently phase-field modelling is a field in which numerical efforts as well as an intense focus on thermodynamic backgrounds and asymptotic behaviour of the models drive the development of this approach.

3. Phase-field models for dislocations

In this section we describe various models, based on the phase field approach, for the simulation of dislocations, their microstructure, their dynamics and the interaction with other objects.

We remark that dislocations pose several challenges for phase field models: (i) it is not immediate that a phase-field approach based on a gradient flow captures the relevant physics. As a note of caution, a fundamental model for the dynamics of a dislocation proposed by Frenkel and Kontorova [50] in 1938 is Hamiltonian,

$$u_j''(t) = u_{j+1}(t) - 2u_j(t) + u_{j-1}(t), -g'(u_j(t)) \quad (5)$$

where u_j is the deformation of the particle j with $j \in \mathbb{Z}$, and g is a periodic on-site potential (the mass is normalised to be 1). This difficulty is not genuine to dislocations but concerns other systems that are microscopically described by Newton's equations of motion (that is, Molecular Dynamics, MD). We return to this point in a moment. (ii) The construction of the free energy F has to account for long-range interaction of dislocations, which results in a nonlocal kernel, such as a double integral. (iii) There is multitude of possible phase field variables, each associated with a slip plane and a slip direction.

As for the reason not to use equations of Molecular Dynamics as in (5), it has to be noted that the time scales achievable in an MD simulation are often insufficient to capture relevant effects for materials. Also, the mathematical analysis of MD can be hard; for example, for the model (5) from 1938, a first rigorous proof for the existence of a dislocation solution was given in 2009 [51], while there is a much more detailed understanding for some of the phase field models discussed below. Other models, such as overdamped dynamics, are often a reasonable approximation in a non-equilibrium situation which is not too far from equilibrium. A justification of approaches using overdamped dynamics, based on a Hamiltonian lattice model, is given in the work by Kresse and Truskinovsky [52]. Also, phase field crystal models can be seen as a time coarse-graining of Molecular Dynamics, as discussed in Subsection 4. Finally, it has recently been shown [53] that an overdamped Frenkel-Kontorova model can be rescaled so that it converges formally to the classic phase

field model by Peierls and Nabarro. The latter is here given by (see [53])

$$\begin{aligned} 0 &= \Delta u^0 && \text{on } \Omega \times (0, \infty), \\ u_t^0 &= 2\epsilon\sigma(\epsilon x_1) - g'(u^0) + \frac{\partial u^0}{\partial x_2} && \text{on } \partial\Omega \times (0, \infty), \end{aligned}$$

where σ is the stress; obviously, this system has to be augmented by an initial condition. Convergence is here understood in the sense that solutions to an overdamped Frenkel-Kontorova model converge formally to a solution of the Peierls-Nabarro model as $\epsilon \rightarrow 0$, where solutions are in both cases understood in the sense of viscosity solutions; a rough sketch of the intuition behind this concept is given in Subsection 3.4.

We note that continuum mechanical phase-field models (PFM) for dislocations commonly use the idea of a phase field which represents the dislocations as platelike inclusions. The phase field thus changes smoothly between two distinct integer values in a region around the interface. This idea distinguishes the continuous models from atomistic (lattice based) models, which describe the dislocation microstructure via segments and/or nodes which are allowed to occupy only certain discrete positions.

We give a brief overview over the key developments for dislocation PFMs, which is a relatively recent field. Léonard and Desai [54] introduced the study of dislocations with PFMs by studying the influence of dislocations on spinodal decomposition. Next, Hu and Chen [55, 56] consider dislocations in a PFM to study solute segregation and nucleation of coherent particles around two-dimensional static edge dislocations. Nabarro [57] noted that a phase-field variable can be used to describe a dislocation loop by analogy to platelike inclusions; this idea was implemented by Wang *et al.* [58] and Rodney *et al.* [59]. The new method, called PFM for dislocations, is an alternative to the line-tracking Dislocation Dynamics [60, 61]. PFMs for dislocations have many attractive features, among them the fact that there is no need to track the evolution of dislocation lines and that simulations can often employ the fast Fourier Transform algorithm, which can be applied to the modeling of anisotropic crystals.

It should be noted that not all further developments of PFMs for dislocations can be related to the standard phase-field model, because they do not use the time-dependent Ginzburg-Landau (TDGL) equation for the evolution of the phase field.

For the sake of the discussion below, we distinguish PFMs for dislocations by introducing different groups, differentiated by the way the dislocation dynamics is simulated and how the elastic problem is solved.

- (1) One group comprises PFMs proposed by Khachaturyan, Wang and coworkers [58, 62, 63]. Here the dislocations loops are labelled by a set of order parameter field variables, similar to coherent misfitting platelet inclusions. Such a description makes it possible to obtain the elastic fields of arbitrary systems of dislocations using the Fourier Transform or more precisely the Khachaturyan-Shatalov (KS) microelasticity theory of the strain of misfitting coherent inclusions [64, 65]. The temporal evolution of the order parameter fields, i.e., the dislocation motion, is described by the TDGL equation. The authors call that an alternative Phase-Field Microelasticity approach. This model was applied further by Hu *et al.* [66] to study the effect of solutes on the dislocation motion. In some sense this model is a pure PFM. The model developed by Kundin *et al.* [67] is also based on the KS

theory. It combines the simulation of the martensitic transformation and the nucleation of transformation dislocations. It uses the TDGL equation for the simulation of the evolution of the martensite phase fields, whereas a phase field of dislocations moves with the moving martensite/austenite boundaries. See Subsection 3.2 for a discussion of the key ideas behind these models.

- (2) A different category are the PFMs developed by Koslowski, Cuitiño and Ortiz [68, 69]. These authors proposed an incremental variational framework, which characterises the evolution of the dislocation by means of a sequence of minimisation problems [70]. For the solution of the elastic problem, the KS microelasticity theory is used. See Subsection 3.3 for a brief survey on these models and related mathematical literature.
- (3) We also mention the model of Alvarez *et al.* [71–73], which relates a phase field with classic dislocation dynamics. More precisely, the authors suggest a level-set method for the calculation of the evolution of the phase field. This model is a variation of the method suggested by Rodney *et al.* [59, 74]. In both models, the authors propose the solution of the problem of the singularity of the strain field on the dislocation line within the scope of the KS theory of microelasticity. See Subsection 3.4.
- (4) There is the approach of phase field crystals, developed by Grant and co-workers. Here the density of the phase field variable, which makes the model atomistic in nature. See Subsection 4 for a discussion.

We recall in the next subsection some basic concepts of micro-mechanical modeling for dislocations which are common to several PFMs. We then discuss the different PFMs mentioned above in the subsequent subsections.

3.1. The eigenstrain and the order parameter

A natural choice for phase field variables is the amount of slip across the crystal plane which separates the slipped and un-slipped region. This is a particular case of the eigenstrain introduced by Eshelby, and we briefly review the key elements in this section. The presentation in this subsection follows [67].

The general analytic theory of the elastic field of a dislocation is developed in many studies [57, 64, 75, 76]. We consider an edge dislocation with Burgers vector b and a slip plane with normal n in a Cartesian coordinate system defined by the cubic lattice. Let the eigenstrain vector of an edge dislocation be given by

$$u_i^d(r, r_0) = b_i H(n\Delta r) H(-e\Delta r), \quad (6)$$

where $H(x)$ is the Heaviside step function,

$$H(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x \leq 0 \end{cases},$$

$\Delta r = r - r_0$ with a site r_0 located on the dislocation line, and $n\Delta r$ and $e\Delta r$ are scalar vector multiplications. The displacement $u_i^d(r, r_0)$ is caused by the relative slip b on the half plane ($n\Delta r = 0$, $e\Delta r < 0$) in the direction of the unit vector in direction of the Burgers vector b , which is perpendicular to a dislocation plane.

In linear elasticity, the strain tensor is given by

$$\epsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i} \right). \quad (7)$$

By substituting (6) in (7), one can see that the eigenstrain tensor of an edge dislocation is of the form

$$\epsilon_{ij}^d(r, r_0) = \frac{1}{2d_0} (b_i n_j + b_j n_i) \delta(n\Delta r) H(-e\Delta r) - \frac{1}{2d_0} (b_i e_j + b_j e_i) \delta(e\Delta r) H(n\Delta r), \quad (8)$$

where $\delta(x)$ is the Dirac delta function. This relation becomes an eigenstrain obtained by Mura [64] in the case $b \parallel x$, $n \parallel y$ and $r_0 = 0$:

$$\epsilon_{12}^*(r) = \frac{1}{2} b \delta(y) H(-x), \quad (9)$$

$$\epsilon_{11}^*(r) = \frac{1}{2} b \delta(x) H(y). \quad (10)$$

The values of the phase field/order parameter, $\phi(r)$, were introduced in PFMs for dislocations [58, 62, 63, 66–69, 73] to describe the amount of inelastic shear of dislocations in units of b . So this parameter replaces the combination of functions $\phi(r) \equiv \delta(n\Delta r) H(-e\Delta r)$ or only the Heaviside function $\phi(r) \equiv H(-e\Delta r)$. Because the phase field changes smoothly in the interface region, the model does not employ a sharp interface approach but describes a diffuse interface model with a width W of the interface. Thus, the question arises how to choose the parameter W in a reasonable way, and (related to this question), how to determine the grid size for simulations, to simulate the real dislocation structure. It is important that the phase field or the order parameter describes the area corresponding to the first term in eq. (8) for the eigenstrain, so that the motion of the dislocation occurs only in a slip plane. The motion in the direction perpendicular to the slip plane is not simulated, assuming that the corresponding probability is small.

A first implementation of the eigenstrain of a dislocation in the phase-field theory was provided by Hu et al. [55]. In this work the authors propose a continuum diffuse interface field model, which couples the Cahn-Hilliard diffusion equation [77] with the elastic fields produced from dislocations. The elastic energy from both compositional inhomogeneities and dislocations is calculated by means of the KS microelasticity theory. The same idea is used in [67] for the calculation of the elastic fields of martensite plates and dislocations. This makes this model different from the approach of Leonard and Desai [54], since the latter uses the analytical solution for the dislocation field. Since the analytical solutions for the elastic fields are not required in KS theory, any complicated defect configurations can be modelled.

Hu et al. [55] use in the simulations the eigenstrain according to the second term in eq. (8) and consider a dislocation loop at the plane perpendicular to a slip plane. A numerical implementation of the Fourier Transform reveals significant oscillations in the stress distributions, caused by the singularity of the eigenstrain. To reduce these oscillations, the authors propose to use a shape function $\Theta(r)$ to describe the eigenstrain, so that the corresponding Fourier transform can be obtained numerically. The difference between the proposed shape function and the phase field $\phi(r)$ used in the models for dislocations reviewed below is that the

function $\Theta(r)$ represents the dislocation loop at the plane described by the Burgers vector and the phase field $\phi(r)$ represents the dislocation loop at the slip plane.

3.2. Time-dependent Ginzburg-Landau approach: phase-field kinetic equation

The standard phase-field kinetic equation derived from the TDGL equation consist of three terms: two terms responsible for the surface energy and a term responsible for the driving force of a transformation. This terms are present in the PFM for dislocations proposed by Wang *et al.* [58]. For simplicity, we write a two-dimensional example of the PFM equation, where there is only one slip plane and one Burgers vector, taken here to be parallel to the x and y axis respectively, and the phase-field $\phi_p(r)$ is confined to the $y = 0$ plane [61]

$$\partial_t \phi_p = k \left[\epsilon (\partial_x^2 + \partial_y^2) \phi_p(x, z) - U \pi \sin[2\pi \phi_p(x, z)] + \sigma_{ij}^{el} e_{ij}^{*p} - \sigma_{ij}^{appl} e_{ij}^{*p} \right], \quad (11)$$

where $e_{ij}^{*p} = \frac{1}{2} b \phi_p$ is the eigenstrain of a dislocation system, the elastic stress σ_{ij}^{el} of dislocation interaction is obtained by the Fast Fourier Transform, and σ_{ij}^{appl} is the externally applied stress. The term responsible for the interaction between dislocations can be written in the form

$$\sigma_{ij}^{el} e_{ij}^{*p} = \sum_k \sum_q B_{pq}(k) \phi_q(k) e^{ikr}, \quad (12)$$

where k are the vectors in reciprocal space ($k_i = 2\pi n_i/L$ with $n_i \in \mathbb{Z}$), and B_{pq} is the interaction matrix between the phases p and q . The first gradient term in eq. (11) is introduced as a part of the core energy of a dislocation, taking into account the dependency on higher order derivatives of the displacement. In [78], it is shown that the gradient term in the form obtained in [79] affects the shapes of the partial peaks and is required for pattern formation in coarse-grained phase-field simulations. Otherwise, there appears an interface width with a surface energy proportional to the area of the dislocation core. The specific of gradient term in the dislocation model is due to the special form of the surface-dependent part of the gradient term, and the remaining length-dependent part can be fitted to describe the dislocation width and the energy of the dislocation core [78]. The second term in eq. (11) is the misfit energy accounting for the non-linear interatomic interactions in the dislocation core. The third term in eq. (11) reproduces the Peach-Koehler force.

In the following we show that the phase-field kinetic equation for dislocation dynamics has a direct analogy to the standard phase-field kinetic equation for the epitaxial growth [80, 81] and at the same time reproduces the ideas of the atomistic Peierls-Nabarro (PN) model of dislocations.

In the originally Volterra model, the discontinuous distribution of a shift vector $u(x)$ (the so-called *misfit distribution function*) across the cut plane of an edge dislocation is presented as a step function. This leads to simple analytical solutions for the elastic fields. However, the solutions for the stress and strain fields (such as the disregistry density $\rho(x) = du(x)/dx$) are singular along the dislocation line. This unphysical behaviour was corrected in the PN model. Here the Burgers vector distribution is spread out with a distribution function to take into account the non-linear interactions in the dislocation core. The analytic solution for the misfit

distribution function $u(x)$ is found as minimizer of the total energy functional

$$E_{tot} = E_{el} + E_{msft}, \quad (13)$$

where

$$E_{el} = \frac{\mu}{4\pi(1-\nu)} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\rho(x')u(x)}{x-x'} dx dx' \quad (14)$$

and

$$E_{msft} = \frac{U}{2} \int_{-\infty}^{\infty} \left[1 - \cos\left(\frac{2\pi u(x)}{b}\right) \right] dx. \quad (15)$$

The corresponding variation in E_{tot} with respect to $u(x)$ must be zero:

$$0 = \frac{\delta E_{tot}}{\delta u} = \frac{\mu}{4\pi(1-\nu)} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\rho(x')}{x-x'} dx' + \frac{U\pi}{b} \int_{-\infty}^{\infty} \sin\left(\frac{2\pi u(x)}{b}\right) dx. \quad (16)$$

The simple analytical solution of this equation is

$$u(x) = \frac{b}{\pi} \arctan\left(\frac{x}{\xi}\right) - \frac{b}{2}, \quad (17)$$

where $\xi = \mu b^2 / (4\pi(1-\nu)U\pi)$ is interpreted as the width of the dislocation core.

We now consider the interface analysis carried out in the standard phase-field model for solidification of a pure substance in [82] and in the phase-field model for the epitaxial growth [80, 81]. The phase-field equation in the model of Liu and Mattioli [80] for epitaxial growth has the form

$$\alpha \epsilon^2 \partial_t \phi = \epsilon^2 \nabla^2 \phi - f_\phi + \lambda g_\phi w, \quad (18)$$

where the standard model functions and their derivatives are $f(\phi) = \frac{1}{\pi}(1 + \cos(2\pi\phi))$, $f_\phi(\phi) = -2\sin(2\pi\phi)$, $g(\phi) = \frac{1}{2\pi}\sin(2\pi\phi) + \phi$ and $g_\phi(\phi) = \cos(2\pi\phi) + 1$. The variable w is the dimensionless density of growth units, which is responsible for the value of the driving force. All three terms in eq. (18) correspond to the three terms in eq. (11) for the dislocations.

In the leading order of a small parameter ϵ the phase-field kinetic equation has the form

$$\partial_\xi^2 \phi - f_\phi = 0. \quad (19)$$

where $\xi = x/\epsilon$ is the inner variable in the standard matched asymptotic analysis. For the canonical choice $f_\phi(\phi) = 2\sin(2\pi\phi)$, which corresponds to the model of Liu and Mattioli [80] for epitaxial growth and the model of Wang *et al.* [58], this equation has the solution for the phase-field

$$\phi(x) = \frac{2}{\pi} \arctan\left(\exp \frac{x\sqrt{\pi}}{W}\right) - \frac{1}{2}, \quad (20)$$

where W is the width of the interface. This analytical form of the phase field derived by Karma and Plapp in [81] for epitaxial growth corresponds to the form of the displacement distribution function in the PN model.

More about the dislocation core structure and the comparison of the PFM of dislocations with the PN model is presented in the reference [3]. Here a quantitative comparison between the so-called microscopic PFM and the PN model is given and a complete agreement of the Burgers vector distribution within the core of an edge dislocation was shown.

Now we move on to the third term of the phase-field equation, which represents the driving forces for the dislocation motion. In the work [66], Hu and coworker suggest the form of the phase field. For the perfect dislocations, $\phi(r)$ should assume integer values inside the dislocation loop and smoothly change on the interface. To satisfy these conditions during a dislocation motion, the driving force term in the phase-field kinetic equation should be transformed. In [66] it was suggested that the function which is used to replace the phase field $\phi(r)$, is of the form

$$f(\phi(r)) = \phi(r) - \frac{1}{2\pi} \sin(2\pi\phi(r)). \quad (21)$$

Here we can see again the analogy to the phase-field model of epitaxial growth. The suggested function $f(\phi(r))$ corresponds to the model function $g(\phi)$, which serves the same aim to keep the integer values inside the phase shape. Note that the new function have to be used only in the term responsible for the driving force.

3.3. Approaches based on energy minimization

In contrast to the standard phase-field model, which uses the TDGL equation for the simulation of the dislocation motion, there are models which rely for this aim on various methods of energy minimization.

The method developed Koslowski *et al.* [68] deserves special attention. Based on the KS theory of microelasticity and the idea of a Peierls misfit potential similar to the model of Wang *et al.* [58], the authors propose an incremental variational method, where the evolution of the phase field is determined by a sequence of minimization problems. The method is a further development of related methods by Ortiz *et al.* [70, 83–85]. The essence of the model is a study of the movement of an ensemble of dislocations within a single slip plane through obstacles, in the presence of applied stress.

The total energy in the model of Koslowski *et al.* [68] for an isotropic medium and the particular case where the Burgers vector points in the direction of the x_1 axis and the slip distribution is confined to the plane $x_3 = 0$ is of the form

$$E(\zeta) = \int \frac{\mu b^2}{2} |\zeta - \xi| dx + \frac{1}{(2\pi)^2} \int \frac{\mu b^2}{4} K |\hat{\zeta}| dk - \int bs\zeta dx, \quad (22)$$

where ξ represents the integer-valued phase-field corresponding to the eigenstrain of the Volterra dislocation, ζ is a normalized slip function, K corresponds to the interaction matrix in the KS theory, and s is the resolved applied stress field. The integrals in (22) are taken over two-dimensional domains. The first term in eq. (22) corresponds to the misfit energy in the Peierls model, the second term is the elastic energy, and the third term is the interaction with the applies stress field. It can be seen that these terms resemble those in the phase-field model of Wang *et al.* [58, 86], with the gradient therm responsible for the evolution of the phase field missing. Instead of this term, the authors use an algorithm for updating the phase-field incrementally.

In comparison to the standard PFM, the automatic evolution of the phase-field by means of a partial differential phase-field kinetic equation is replaced by the series of

incremental updates. Unlike some standard PFMs, which are three-dimensional, the model [68] considers a two-dimensional dislocation distribution, and the energetic expression of the misfit energy is less complex. This makes the two approaches rather different; the reduction of complexity in [68] is intentional, the motivation being to make the model analytically tractable by using analytic expressions, and thus reduce the computational effort.

An extension of this model to slip process's with activation of multiple slip systems is given in [69], and the model is used there to study twist boundaries of finite extent.

The variational nature of the incremental updates have the advantage that tools from the calculus of variations can be used. Of particular interest from a mathematical perspective is the possibility to study suitable limits of the associated functionals. Gamma-convergence is an appropriate notion of convergence of functionals. We state a suitable (sequential) definition of Gamma-convergence; a detailed presentation can be found in the books by Braides [87] and Dal Maso [88]. If $\{E_n\}_{n \in \mathbb{N}}$ is a sequence of functionals (for example, the energy discussed above, under a scaling linked to n), then E_n Γ -converges in a suitable space X to the functional E , denoted $E_n \xrightarrow{\Gamma} E$ as $n \rightarrow \infty$, if the following two conditions hold true:

- (1) (Lower bound) For every $u \in X$ and for every $u_n \rightarrow u$ in X we have

$$\liminf_{n \rightarrow \infty} E_n(u_n) \geq E(u).$$

- (2) (Recovery sequence) For every $u \in X$, there exists a sequence $\{u_n\}_{n \in \mathbb{N}} \subset X$ such that $u_n \rightarrow u$ and

$$\limsup_{n \rightarrow \infty} E_n(u_n) \leq E(u).$$

Naïvely speaking, the lower bound shows that E is an approximation “from below”, which is important for arguments based on energy minimization as here the incremental problems, and the recovery sequence shows that this bound is sharp in the sense that it is attained.

In a periodic setting, the Peierls potential can be taken to be $\frac{1}{\epsilon} \int_T \text{dist}^2(\xi(x), \mathbb{Z}) dx$ (that is, noninteger values of the slip in measured in units of the Burgers vector are penalised; T denotes the flat torus $\mathbb{R}^2/\mathbb{Z}^2$) for a long-range elastic energy $\frac{1}{2} \int_T \int_T K(x - x') |\xi(x) - \xi(x')|^2 dx dx'$ (here written in real space), Garroni and Müller [89] have shown that the sum of this Peierls potential and this elastic energy, scaled suitable, Gamma-converges as $\epsilon \rightarrow 0$ to a functional which can be called a dislocation capacity (there are various technical aspects which we cannot discuss here; a flavour of the result has to suffice here, and we remark that the limit has a physical interpretation, namely that of a large body limit).

A vectorial version of the aforementioned scalar result is as follows. The functional

$$E_\epsilon(\xi) = \frac{1}{|\log \epsilon|} \int_T \int_T (\xi(x) - \xi(x'))^T K(x - x') (\xi(x) - \xi(x')) dx dx' + \frac{1}{\epsilon |\log \epsilon|} \int_T \text{dist}^2(\xi(x), \mathbb{Z}^n) dx \quad (23)$$

(with ξ being a one-periodic vector field and K a suitable kernel) Gamma-converges

to the functional

$$E(\xi) = \int_{S_\xi} \phi([\xi], n_\xi) d\mathcal{H}^1,$$

where S_ξ denotes the jump set of ξ in the domain, n_ξ is the normal vector of S_ξ and $[\xi]$ denotes the jump of ξ ; ϕ is a density function whose existence is part of the theorem. This result is due to Cacace and Garroni [90]. As in the previous discussion of Gamma-convergence results, we have to gloss over a number of subtle issues (for example, the definition of the functional E_ϵ is valid only for suitable functions ξ and best thought of to be ∞ otherwise; same for the limiting functional). Yet, seems important to point out that these abstract results offer relevant mechanical insight: the limit $\epsilon \rightarrow 0$ in [90] is an anisotropic line tension model for line defects. A key feature of Gamma-convergence is that for a sequence of functionals, their minima converge under very natural assumptions to the minimum of the Gamma-limit, here the anisotropic line tension model. For the functionals (23) associated with the PFM (and their modifications including lower-order terms such as applied stresses), this means that their minimization can in the limit be replaced by the minimization of the line tension model. Furthermore, the proof of a Gamma-convergence result often offers interesting insight. For example, in [90] it is shown that flat interfaces are in general not optimal in the case of the functional (23); instead, the proof reveals that a sequence of transitions resulting in interfacial microstructure is energetically favourable.

3.4. Models combining a phase field with classic dislocation dynamics

Another interesting approach for the investigation of dislocation dynamics in the framework of a phase field model is the Hamilton-Jacobi approach developed by Alvarez *et al.* [72, 73]. In this method, the dynamics of a single dislocation line is described by an Hamilton-Jacobi equation, equivalent to classical dislocation dynamics (the motion of dislocations in a crystal is governed by a nonlocal eikonal equation, where the velocity is a function of elastic fields generated by the dislocations).

This method builds on the PFM proposed by Rodney *et al.* [59, 74]. The key question is here how to describe the dislocation core appropriately, and we discuss a few approaches concerned with this topic.

3.4.1. The dislocation core in a phase-field model

The problem of how to obtain a realistic description of the dislocation core in a PFM has been studied by many authors. The use of a diffuse-interface approach in the simulation of the dislocation motion leads to a very wide core, which is associated with the width of the interface. This value does not match experimentally determined cores. Since the core radius controls the maximum stress near dislocations and thus the short-size interaction between the dislocations and concentration fields, the need a new scheme for the simulation at the nanoscale is apparent.

A first solution of this problem was suggested by Rodney *et al.* [74]. These authors present an improved version of the phase-field model of Wang *et al.* [58], taking into account the Angström-scale dislocation core in a microscale simulation cell. The model maintains the generality of the original model as far as the KS microelasticity theory [65] is concerned. In the framework of this theory, the authors suggest the decomposition of a dislocation loop into a superposition of elementary so-called *loopons*. Consequently, a dislocation phase-field is decomposed into a sum of fields of loopons, so that the shape function Θ_p (which is 1 if the point is in phase p and

0 otherwise) is decomposed,

$$\Theta_p(r) = \sum_n \Theta_p^d(n) S_p(r - r_n), \quad (24)$$

where n runs over all grid points, S_p is the shape function of a loopon,

$$S_p(r) = H_{\frac{a}{2}}(x) H_{\frac{a}{2}}(y) H_{\frac{a}{2}}(z - d/2), \quad (25)$$

with $H_l(x) = 1$ if $|x| < l$ and 0 otherwise, d being the lattice size and a being the core size.

This approach introduces a second independent scale to a PFM, associated with the dislocation core. Mathematically, it can be expressed by replacing the interaction matrices, which are part of the Fourier transform in the elastic energy equation (12), by so-called *decorated matrices*:

$$B_{pq}^{dec}(k) = \sum_g B_{pq}(k + g) S_p(k + g) S_p^*(k + g), \quad (26)$$

where $k_i = 2\pi n/Nd$ with $n \in [-N/2, N/2]$ is the vector of the first Brillouin zone and $g_i = 2\pi m/d$ with $m \in \mathbb{Z}$ is the vector of the reciprocal lattice. Physically, the decorated interaction matrices correspond to the Fourier transform of the interaction energy of a pair of loopons belonging to the systems p and q .

To avoid very wide dislocation cores, Rodney *et al.* [74] use for the simulation of the dislocation dynamics a discrete algorithm, where dislocation phase fields vary discretely from one integer to other one. The algorithm is based on the motion of the dislocation segments that border the loops. This segments are displaced proportional to the driving force as in classical Discrete Dislocation Dynamic [91].

The problem of the width of the dislocation core is also addressed in the model of Alvarez *et al.* [72]. The authors suggest a *core distribution function*, χ_0 , to remove the singularity of the strain field on the dislocation line. The Fourier transform of the core function, which is matched to the Peierls model, has the form

$$\hat{\chi}_0(\xi_1, \xi_2) \sim e^{-\frac{\zeta}{2} \sqrt{\xi_1^2 + \xi_2^2}}, \quad (27)$$

with ζ a parameter corresponding to the core size.

We remark that a similar approach to the problem of the singularity of stress field on the dislocation line was taken in the work of Hu and Chen [55]. To reduce the oscillations in the dislocation stress field calculated by the Fast Fourier Transform, it is proposed there to use Gaussian functions to describe the Burgers vector distribution

$$b_i = b_{i0} \frac{\alpha_1 \alpha_2}{\pi} e^{-[\alpha_1^2 (x-x_0)^2 + \alpha_2^2 (y-y_0)^2]}, \quad (28)$$

where (x_0, y_0) is the centre of the distribution and α_i are coefficients responsible for the localisation of the distribution.

It is apparently that in the PFM of Wang *et al.* [58], the singularity does not exist since the step function of the eigenstrain of the Volterra dislocation is replaced by a continuous phase field function. Moreover in this PFM, as in the methods presented in this subsection, the precision of simulations depends on the choice of the size of the dislocation core, which corresponds to the size of the discretization grid in the numerical simulation.

More about the dislocation core structure and the comparison of PFMs of dislocations with the PN model is presented in the reference [3]. Here, a quantitative comparison between the so-called microscopic PFM and the PN model is given and a complete agreement of the distribution of the Burgers vector within the core of an edge dislocation is shown.

3.4.2. A Hamilton-Jacobi approach and its level set formulation

We now return to the discussion of the model derived by Alvarez *et al.* [72]. Here, the dynamics of a single dislocation line Γ is described by a Hamilton-Jacobi equation.

The core tensor plays a central role in this model. With the choice (27), the core tensor χ_{ijkl} is

$$\chi_{ijkl} = \chi_0(x_1, x_2) \delta_0(x_3) \frac{1}{2} (\delta_{ij} \delta_{kl} + \delta_{jk} \delta_{il})$$

(with x_3 being in the direction of the slip plane normal, and the dislocation moving in the plane; $\delta_0(x_3)$ is a Dirac mass only in x_3 direction). A dislocation loop is described by a discontinuous field Θ which is 1 inside the loop and 0 outside. That is, Θ is the characteristic function of a two-dimensional domain Ω , $\Theta = 1$ on Ω and $\Theta = 0$ on $\mathbb{R}^2 \setminus \Omega$. The physical strain is then given by the convolution

$$\epsilon_{ij} = \chi_{ijkl} \star (\rho \delta_0(x_3) \epsilon_{kl}^0) + \epsilon_{ij}(U),$$

where U is a three-dimensional displacement vector, $\epsilon(U)$ its associated linear strain. This smoothing gives, for χ_{ijkl} smooth enough and energy-minimising U , in a natural way rise to a well-defined line energy of the usual form

$$E(\Gamma) = \frac{1}{2} \int_{\mathbb{R}^3} \lambda_{ijkl} \epsilon_{ij} \epsilon_{kl}.$$

The authors define the Peach-Koehler force $c = c_0 \star \Theta$ using the method of Green's functions. Then the evolution of $\Theta = \Theta(x_1, x_2, t)$ is given by a nonlocal Hamilton-Jacobi equation,

$$\frac{\partial \Theta}{\partial t} = c |\nabla \Theta|,$$

which is an equivalent of classically dislocation dynamics.

As a characteristic function, Θ is discontinuous, and it is advantageous to localise the dislocation in the spirit of level sets, that is, as the zero set of a function $u = u(x_1, x_2, t)$, where the dynamics of u is given by

$$\frac{\partial u}{\partial t} = (c_0 \star H(u)) |\nabla u|, \quad (29)$$

with H the Heaviside function. Equation (29) is to be supplemented by the initial condition $u(x_1, x_2, 0) = u^0(x_1, x_2)$.

This approach makes level set methods a natural approach for the study of the evolution of dislocation lines which are graphs or closed loops. In particular, the phase field approach simplifies the analysis of topological changes during a movement of a dislocation. However, the analysis of (29) is far from trivial, due to the dependence of the velocity on the solution itself.

The governing equation's nature as nonlocal Hamilton-Jacobi equation makes a rich toolbox of relatively recent mathematical advances available, both numerically and analytically.

We first sketch the analytic properties. The governing kinetic equation (29) has in general not a unique solution. This is common for Hamilton-Jacobi equations; Crandall and P. L. Lions developed the theory of viscosity solutions to single out solutions. For Hamilton-Jacobi equations, an interpretation of this solution concept based on viscous regularisations can be made; the theory has since been extended to cover a wide range of equations, notably degenerate elliptic and parabolic equations. In a nutshell, viscosity solutions apply to *degenerate elliptic* equations, which are equations

$$E(u, Du, D^2u) = 0$$

(with $u: \Omega \rightarrow \mathbb{R}$, Du being the first and D^2u being the second derivative) such that

$$E(r, p, X) \leq E(r, p, Y) \quad \text{if } Y \leq X \quad (30)$$

for every admissible r and p . As a rather trivial example, the elliptic equation $-u''(x) = f$ (note the minus sign!) is degenerate elliptic. Viscosity (super- and sub-) solutions are then solutions which are continuous but not necessarily any smoother; they are singled out of the multitude of possible solutions by a comparison with twice differentiable functions lying above or below the solution candidate. A rough intuition is that in principle, for degenerate elliptic equations, suitable solution segments can be pieced together to give rise to new solutions; the comparison with smoother functions singles out the admissible non-smooth transitions. For parabolic equations, time is added as additional spatial variable. We refer the reader to the beautiful survey [92] for in-depth information in a very readable presentation.

For (29), it is possible to prove a local (that is, short time) existence and uniqueness result for the solution, in the context of viscosity solutions [93].

The computation of a solution can be based on the framework of level set methods by Osher and Sethian. Specifically, in [93], the authors propose a numerical method based on a monotone numerical Hamiltonian proposed by Osher and Sethian. This leads to a first order finite difference scheme for the level set formulation (29). The convergence of this scheme can be proved, as well as an estimate of the rate of convergence $O(\sqrt{\Delta t})$ [93]. A number of numerical simulations in a periodic setup can be found in the same reference. In comparison to some other PFMs, an advantage is that rigorous statements on the convergence of numerical methods can be made; on the other hand, [72] is confined to the motion of a single dislocation line.

4. The phase field crystal method

The phase field crystal (PFC) model proposed by Elder *et al.* [15] is a new extension to phase-field modeling which introduces a field for the atomic density of the material, with the aim of allowing long-time simulations for out of equilibrium situations at the microscopic scale. The evolution of the density is described according to dissipative dynamics with driving force derived from the free energy minimization.

An general feature of this approach is that it resolves, by construction, the microscopic structure while being computationally cheaper than a full Molecular Dyna-

mics simulation (MD). An interpretation of phase field crystals as temporal coarse-graining to MD is available [94], sketched below.

Let ρ here be the order parameter corresponding to the density. The energy is

$$F = \int \left[\frac{\rho}{2}(\epsilon + (1 + \Delta)^2)\rho + \frac{\rho^4}{4} \right] dx,$$

where ϵ is a phenomenological constant (which can be related to temperature). The dynamics is

$$\frac{\partial \rho}{\partial t} = \Delta \frac{\partial F}{\partial \rho} + \xi, \quad (31)$$

where ξ is a Gaussian random noise. As can be seen from (31), the dynamics is diffusive and does not capture effects happening on fast time scales. Yet, in principle the dynamics could be compared to the time averaged microscopic dynamics; another attractive feature if this approach is that the energy functional can be derived from density functional theory. As it was shown in the work of Elder *et al.* [95] specifically, in density functional theory for freezing of pure and binary systems, the free energy functional is expressed in terms of the time averaged atomic density field. It can then be expanded around a liquid reference state (along the liquid-solid coexistence line). This yields an expansion in terms of n -point correlation functions; if one considers then a cut-off such as the pair correlations, then the resulting free energy can be matched to a PFC model. Thus, the PFC model can be viewed as a simplified form of density function theory in the sense that the parameters of the PFC model can be related to the physical constants of the density functional theory framework.

The PFC model differs from other phase-field approaches in that in equilibrium, the constructed phase field (the time-averaged density) is periodic, mimicking a perfect crystalline structure. This periodic form naturally describes the elastic effects, misfits on the grain boundaries, nucleation and motion of dislocations. In the work [97] Elder and Grant show that the elastic and plastic effects are naturally included in the PFC model. The free energy functional of the form (4) can be written by using a periodic field (the simple example is $\rho(x) = A \sin(2\pi x/a)$) in Hook's low form, linked the formalism to the classical microelastic theory. This feature was exploited for the simulation of elastic and plastic effects.

Within the framework of PFC, dislocation processes such as glide, climb, and annihilation was studied in the work of Berry *et al.* [96]. An initial density corresponding to a single edge dislocation is prepared in the hexagonal state [97]

$$\rho(x, y) = A \left[\cos\left(\frac{2\pi x}{a\sqrt{3}}\right) \cos\left(\frac{2\pi y}{a\sqrt{3}}\right) - \frac{1}{2} \cos\left(\frac{4\pi y}{a\sqrt{3}}\right) \right] + \rho_0, \quad (32)$$

where ρ_0 is the average density, a is the lattice constant and A is defined by the energy minimization. Then (31) is solved by time discretization and a spherical Laplacian approximation in space, in a two-dimensional periodic setting. Two stable dislocation configurations are found in equilibrium, and it is shown that the Peierls barriers for glide and climb is relatively insensitive toward the dislocation density. The model exhibits both elastic and plastic behavior, the latter in the form of Peierls potentials, without having incorporated these effects *a priori*. PFC is a versatile method to study atomistic effects, which is a different focus from the other dislocation PFMs discussed in this article.

The dislocation nucleation and motion by spinodal decomposition were studied by many authors within the PFM [54, 55] and withing the coupling of the PFM/PFC models [98]. In the work [95] the spinodal decomposition in binary alloys was studied within the PFC by using the two-point correlation functions and the rescaled density. The simulations contain compositional domain boundaries and grain boundaries between grains of different orientations. It was shown that the observed dislocation motion is affected by elastic strain energy due compositional differences arising during the phase separation.

Recently the phase field crystal method has been applied to a variety of different growth phenomena. Amongst these are for example liquid phase epitaxy [15], material hardness [15, 21] and eutectic growth [17, 18]. In the context of the latter article the approach could be extended to binary alloys. Other further developments concerned the coupling of phase-field and phase-field crystal method via renormalisation [12, 13]. Also applications to heterogeneous nucleation have been developed [111].

We now sketch the interpretation of PFCs as coarse-grained Molecular Dynamics. Tupper and Grant [94] consider the usual model of Molecular dynamics, with the Hamiltonian

$$H = \sum_{j=1}^N \frac{p_j^2}{2m} + V(r_1, \dots, r_N),$$

describing the energy associated with the positions r_j and the momenta p_j of N particles of constant mass m in the plane. Here V can be taken to be the Stillinger-Weber potential, which augments a Lennard-Jones type of potential with three-body interactions. Then, if $\rho_m(r, t) = \sum_{j=1}^N \delta(r - r_j(t))$ is the microscopic density, a temporal coarse-grained version is, for some $\tau > 0$,

$$\rho(r) = \frac{1}{\tau} \int_0^\tau \rho_m(r) dr.$$

Tupper and Grant derive a PFC model for the dynamics of the coarse-grained density field ρ , where τ is large but finite. The energy again builds on correlation functions originating from density function theory. The temporal evolution is a diffusion equation with noise, or alternatively a stochastic version of a phase-field type of equation. A numerical comparison with time-averaged Molecular Dynamics shows a good agreement, as discussed in [94]. In this sense, the theory of PFCs can be interpreted as a coarse-grained version of Molecular Dynamics.

5. Concluding outlook: Multiscale modelling of dislocation dynamics involving phase-field and phase-field crystal approach

Fig. 1 shows that there is an inherent challenge to the simulation-based study of coupled phase and structure evolution problems in materials science, such as dislocation dynamics, to which phase-field and phase-field crystal models can be applied: The latter is essentially a multi-scale dynamics, i.e., a dynamics where different evolution paths occurring at different length and time scales are strongly coupled to each other. The examples discussed in Section 1 point this out more illustratively for the topic of this review, dislocation dynamics. As outlined there, a truly multiscale approach for problems of dislocations dynamics in materials science should grasp important features from the microscopic as well as the atomic scale.

In this context, it is worth noticing that due to the continuum field nature of the phase-field approach, one can claim that it should not be valid in the nano-scale region. However, due to the successes of continuum approaches in nano-fluidics, it appears to be justifiable to proceed with phase-field models for phase transition problems of similar physical nature at this scale as well. Indeed, successful studies have been carried out already [99] and give a thorough foundation for future work.

With this background, it is quite easy to understand that in the further development of the phase-field and the phase-field crystal method in the context of computational materials design, a lot of activities are concerned with this ‘scale-bridging’ issue, in particular now that a combination of these methods allows to directly couple the atomic scale to the microscale. In multiscale modeling based on phase-fields, basically three avenues have emerged in the community. The first is to design innovative algorithms which couple different computational techniques, originally designed for complementary scales as, e.g., DLA (Diffusion Limited Aggregation) [100], LBA (Lattice Boltzmann Automata) [101] or MC (Monte Carlo) schemes [102], to a phase-field model. The second is to use advanced numerical techniques such as multi-grid, adaptivity and parallelisation to carry out fast computation on several scales based on a single model approach [103–105]. A third possibility arises from analysis, i.e., rigorous homogenisation methods where one identifies the most relevant dynamical processes at each scale and develops a scale-bridging model based on these via expansion techniques [106].

With respect to the first avenue, the coupling of different computational techniques originally designed for complementary scales, one has to distinguish two approaches: The first is the calculation of physical quantities which are determined at lower scales of the overall simulation and can assumed to be constant during the simulation at the larger scales, *a priori* to insert them into the larger scale simulations as fixed parameters. This has sometimes been termed *weak coupling*, whereas the opposite discussed below is often referred to as *hard* or *full dynamic coupling*. A very general multi-scale first-principle/phase-field method following a *weak coupling* concept has recently been developed in [107]. Apart other things, it can also be applied to dislocation dynamics. *Hard* or *full dynamic coupling* means to couple the different techniques dynamically, such that in every time step of the overall algorithm calculations with both methods are carried out and well-defined quantities are continuously evaluated and exchanged across the scales. The examples above [100–102] fall in this category. From a computational point of view, this is still very demanding and possible only for carefully selected problems. Homogenisation as well as renormalisation methods can help to establish more models of this kind in the future. Among the two, in particular the renormalisation concept has proven to be quite successful in coupling the phase-field and the phase-field crystal approach [12, 13] to a full dynamic approach, reaching from the atomic scale to the microscale. From the point of view of materials engineering, this is exactly an approach that would tackle challenges as discussed in Section 1 for dislocation dynamics. Thus it is a very promising concept, especially for the multiscale modeling of dislocation dynamics. This is in particular true since other than in phase-field modeling, where a developing a model to describe dislocations dynamics is tied to conceptional challenges (see Section 3), in phase-field crystal modeling a concept of dislocations arises inherently [15]. Via renormalisation, this concept could then also be ‘transported’ to the microscale. Several steps are still open to truly develop a comprehensive, scale-bridging model approach along these lines which allow to treat dislocation dynamics and successively more complex problems of deformation mechanics in a versatile manner: First, since in the simplistic PFC model the material is defined by only three parameters, it is restricted with respect to the crystal

lattice structures which it can describe. These are triangular symmetries in two dimensions and *BCC* symmetry in three dimensions [108]. Another crystal symmetry appearing in protein crystals in a membrane could be obtained by including higher order correlation functions [109]. Moreover, liquid crystals have been simulated by combining the original phase-field crystal equation with an orientational field [110]. More recently, an anisotropic generalisation of the phase-field crystal method has been developed by one of the authors and coworkers [111]. However, the full investigation of its phase diagram is still work in progress. Second, the computational load of such a model will be highly demanding and sophisticated schemes such as adaptivity [12, 13] are likely to be required. However, due to the high relevance in terms of impact for materials science in general, we would like to conclude by stating that further steps along this direction would be relevant and promising.

Literatur

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